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INTRODUCTION

In a stochastic medium, the material properties at a given spatial location are known only statistically [1]. The most common approach to solving particle transport problems involving binary stochastic media (BSM) is to use the atomic mix approximation [1] in which the transport problem is solved using homogenized (volume-averaged) material properties. A common deterministic model developed for solving BSM particle transport problems is the Levermore-Pomraning (LP) model [1, 2]. Zimmerman and Adams [3] proposed a Monte Carlo algorithm (Algorithm A) that solves the LP equations and another Monte Carlo algorithm (Algorithm B) that locally preserves the sampled material realization [3, 4]; we refer to these Monte Carlo algorithms as the LP and LPLRP (LP local realization preserving) algorithms, respectively. One-dimensional (1D) planar geometry benchmark studies have shown that the LPLRP algorithm is often significantly more accurate than the LP algorithm for problems with an incident angular flux [3, 4] as well as for problems with an interior source [4]. The LPLRP algorithm implementation in these benchmark comparisons made explicit use of the one-dimensional nature of the problem.

The LP model is derived by assuming an "upwind" closure in the coupling term relating the two materials in a binary stochastic medium [5]. Su and Pomraning [6] developed a modified form of this closure by considering the small correlation length limit and requiring the modified closure to produce the correct exponential decay for a source-free halfline albedo problem in rod geometry. They concluded that the modified closure is generally not inferior to the LP closure and in some cases is significantly better [6]. Brantley [7] investigated the use of the Su-Pomraning (SP) closure in the Monte Carlo LP algorithm (LP-SP) for the suite of benchmark problems described in [4] and concluded that 1) the LP-SP algorithm was somewhat more accurate overall than the LP algorithm and somewhat less accurate overall than the LPLRP algorithm for an incident angular flux benchmark suite, and 2) the LP-SP algorithm was generally the least accurate of the algorithms for an interior source benchmark suite.

Larsen et al. [8] performed an asymptotic analysis of the transport equation in 1D planar geometry for the situation in which the physical system is 1) a random binary stochastic medium with material macroscopic total cross sections and mean slab width values of $O(1)$ or smaller and 2) optically thick with weak absorption and sources at each spatial point and therefore globally diffusive. The asymptotic analysis demonstrates that, under these assumptions, the transport equation limits to the conventional diffusion equation with atomically-mixed (volume-averaged) material properties. Larsen et al. [8] also demonstrate that, under these same assumptions, the LP equations asymptotically limit to an atomically-mixed diffusion equation with a diffusion coefficient that is too large, leading to an unphysical flattening of the ensemble-averaged scalar flux distribution. Vasques and Yadav [9] recently performed an asymptotic analysis of an adjusted Levermore-Pomraning closure in which the Markovian transition functions are rescaled such that the equations asymptotically limit to the correct atomically-mixed diffusion equation; we refer to this model as LP-VY.

In this paper, we demonstrate that the adjusted LP closure proposed by Vasques and Yadav [9] is a special case of the SP closure obtained by assuming that the absorption cross sections in the two materials are equal. We further demonstrate that the Su-Pomraning closure has the correct asymptotic limit for the diffusive physical system considered in [8, 9] and is therefore an appropriate closure for these problems. We also describe how to incorporate these various closures into the Monte Carlo LP and LPLRP particle transport algorithms, and we present numerical results comparing the accuracy of the Monte Carlo LP, LP-VY, LP-SP, LPLRP, and LPLRP-SP algorithms for the set of diffusive benchmark problems in [9].

DIFFUSIVE BINARY STOCHASTIC MEDIUM TRANSPORT PROBLEMS

We consider the following time-independent monoenergetic particle transport problem [4] with isotropic scattering in a one-dimensional planar geometry spatial domain:

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\Sigma_t(x)\psi(x,\mu)=$$
$$\frac{1}{2}\Sigma_s(x)\int_{-1}^{+1}\psi(x,\mu')\,d\mu'+\frac{1}{2}Q(x)\ ,$$
$$-X\le x\le X\ ,\ -1\le\mu\le 1\ , \tag{1}$$
$$\psi(-X,\mu)=0\ ,\ \mu>0\ , \tag{2}$$
$$\psi(X,\mu)=0\ ,\ \mu<0\ . \tag{3}$$

Eqs. (1)–(3) are written in standard neutronics notation [10]. When the cross sections are random variables, the angular flux is also a random variable. The vacuum boundary conditions given by Eqs. (2) and (3) are non-stochastic.

The binary stochastic spatial medium is assumed to be composed of alternating slabs of two materials, labeled with the indices 0 and 1, with the mean material slab width for material i denoted as Λ_i. The total and scattering cross sections for each material are denoted as $\Sigma_{t,i}$ and $\Sigma_{s,i}$, $i=0,1$, respectively. The distribution of material slab widths in the planar medium is assumed to be described by spatially homogeneous Markovian statistics [1], in which case the slab width values for material i, λ_i, follow an exponential distribution given by

$$f_i(\lambda_i)=\frac{1}{\Lambda_i}\exp\left(-\frac{\lambda_i}{\Lambda_i}\right)\ , \tag{4}$$

where again Λ_i is the mean material slab width for material i. Given the mean material slab widths, the probability of finding material i at any given spatial point, p_i, is given by

$$p_i = \frac{\Lambda_i}{\Lambda_0 + \Lambda_1} \quad . \tag{5}$$

This material probability corresponds to the volume fraction of the material in the problem. The ensemble average of any macroscopic cross section value is given by

$$\langle \Sigma_x \rangle = p_0 \Sigma_{x,0} + p_1 \Sigma_{x,1} \quad . \tag{6}$$

The generalized LP model for this binary stochastic medium transport problem is

$$\begin{aligned} &\mu \frac{\partial}{\partial x} \left[p_i \psi_i (x, \mu) \right] + \Sigma_{t,i} p_i \psi_i (x, \mu) = \\ &\frac{1}{2} \Sigma_{s,i} \int_{-1}^{+1} p_i \psi_i (x, \mu') \, d\mu' + \frac{1}{2} p_i Q_i \\ &+ \Theta |\mu| \left[\frac{p_j \psi_j (x, \mu)}{\Lambda_j} - \frac{p_i \psi_i (x, \mu)}{\Lambda_i} \right] \quad , \\ &-X \leq x \leq X \quad , \quad -1 \leq \mu \leq 1 \quad , \end{aligned} \tag{7}$$

for the material index $i = 0, 1$ and $j \neq i$. Here $\psi_i (x, \mu)$ is the material i angular flux at spatial location x in direction μ. The parameter Θ is a general multiplier on the Markovian transition functions that can be used to implement various closure models. Setting the multiplier $\Theta = 1$ in Eq. (7) produces the standard LP model.

Su-Pomraning (SP) Closure

Su and Pomraning [6] derived the following equation for a closure multiplier Θ_{SP} by requiring the LP model with the modified closure to give the correct exponential decay for a source-free halfline albedo problem in rod geometry:

$$\Theta_{SP} = \frac{\sqrt{\langle \Sigma_a \rangle \langle \Sigma_t \rangle} \left[\langle \Sigma_a \rangle (\Sigma_{t,1} - \Sigma_{t,0})^2 + \langle \Sigma_t \rangle (\Sigma_{a,1} - \Sigma_{a,0})^2 \right]}{\left[\langle \Sigma_a \rangle (\Sigma_{t,1} - \Sigma_{t,0}) \right]^2 + \left[\langle \Sigma_t \rangle (\Sigma_{a,1} - \Sigma_{a,0}) \right]^2} \quad , \tag{8}$$

where $\Sigma_{a,i} = \Sigma_{t,i} - \Sigma_{s,i}$ is the absorption cross section for material i, and the ensemble-averaged absorption cross section is computed as $\langle \Sigma_a \rangle = p_0 \Sigma_{a,0} + p_1 \Sigma_{a,1}$. For a purely absorbing medium, $\Theta_{SP} = 1$ and the LP approximation (exact in a purely absorbing medium) is recovered. Setting $\Theta = \Theta_{SP}$ in Eq. (7) produces the LP-SP model.

Vasques-Yadav (VY) Closure

Extending the work of Larsen et al. [8], Vasques and Yadav [9] investigated another form for a closure multiplier Θ_{VY} using a multiple length-scale asymptotic analysis. They assumed the physical system is 1) a random binary stochastic medium with material macroscopic total cross sections and mean slab width values of $O(1)$ or smaller and 2) optically thick with weak absorption and sources at each spatial point and therefore globally diffusive. These assumptions imply that the number of material slabs in the system is large.

Assuming the physical system is optically thick, they defined a small dimensionless parameter ϵ as

$$\epsilon = \frac{\text{mean width of material slab}}{\text{width of system}} = \frac{1}{\text{number of slabs}} \quad . \tag{9}$$

Assuming that absorption and the interior source are weak at all spatial points, they scaled the macroscopic absorption cross section as

$$\Sigma_a (x) = \Sigma_t (x) - \Sigma_s (x) = \epsilon^2 \sigma_a (x) \quad , \tag{10}$$

and the interior source as

$$Q (x) = \epsilon^2 q (x) \quad , \tag{11}$$

where $\sigma_a (x) = O(1)$ and $q (x) = O(1)$. As a result of these scalings, the infinite-medium scalar flux solution

$$\phi (x) = \int_{-1}^{+1} \psi (x, \mu) \, d\mu = \frac{Q (x)}{\Sigma_a (x)} = \frac{q (x)}{\sigma_a (x)} \tag{12}$$

is $O(1)$. Under these assumptions, Larsen et al. [8] and Vasques and Yadav [9] demonstrate using a multiple length-scale asymptotic analysis that Eq. (1) asymptotically limits to the correct conventional diffusion equation

$$-\frac{1}{3 \langle \Sigma_t \rangle} \frac{d^2}{dx^2} \phi (x) + \langle \Sigma_a \rangle \phi (x) = \langle Q \rangle \quad , \quad -X \leq x \leq X \quad , \tag{13}$$

with atomically-mixed (volume-averaged) cross sections.

To proceed with the asymptotic analysis of the LP equations, Eq. (7), Vasques and Yadav first assumed that the material macroscopic total cross sections $\Sigma_{t,i}$ and mean material slab width values Λ_i are $O(1)$. Then assuming that absorption and interior sources are weak in both materials, they scaled the material macroscopic absorption cross sections as

$$\Sigma_{a,i} = \Sigma_{t,i} - \Sigma_{s,i} = \epsilon^2 \sigma_{a,i} \quad , \tag{14}$$

where $\sigma_{a,i} = O(1)$, and the material interior sources as

$$Q_i = \epsilon^2 q_i \quad , \tag{15}$$

where $q_i = O(1)$. Under the general assumption that Θ_{VY} is $O(1/\epsilon)$, they proceeded to demonstrate that Eq. (7) asymptotically limits to the correct conventional diffusion equation with atomic mix (volume-averaged) cross sections given by Eq. (13). Motivated by this asymptotic analysis, Vasques and Yadav defined the multiplier Θ_{VY} to be

$$\Theta_{VY} = \sqrt{\frac{\langle \Sigma_t \rangle}{\langle \Sigma_a \rangle}} \quad . \tag{16}$$

This form of the multiplier has the desirable properties that 1) $\Theta_{VY} = O(1/\epsilon)$, resulting in the correct asymptotic diffusion behavior, and 2) $\Theta_{VY} = 1$ when $\langle \Sigma_a \rangle = \langle \Sigma_t \rangle$, resulting in the correct LP approximation for a purely absorbing medium. However, we note that this multiplier definition was motivated by the asymptotic analysis but is not directly produced by the asymptotic analysis. Setting $\Theta = \Theta_{VY}$ in Eq. (7) produces the LP-VY model.

Relationship Between SP and VY Closures

Following some minor algebraic manipulation, the Su-Pomraning closure Eq. (8) can be related to the Vasques-Yadav closure Eq. (16) as follows:

$$\Theta_{SP} = \Theta_{VY} \frac{1 + \Theta_{VY}^2 \left(\frac{\Sigma_{a,1}-\Sigma_{a,0}}{\Sigma_{t,1}-\Sigma_{t,0}}\right)^2}{1 + \Theta_{VY}^4 \left(\frac{\Sigma_{a,1}-\Sigma_{a,0}}{\Sigma_{t,1}-\Sigma_{t,0}}\right)^2} \quad . \tag{17}$$

If we make the assumption that the macroscopic absorption cross section is equal in both materials, $\Sigma_{a,0} = \Sigma_{a,1}$, we find that

$$\Theta_{SP} = \Theta_{VY} \quad . \tag{18}$$

As a result, we conclude that the Vasques-Yadav closure is a specific case of the Su-Pomraning closure that assumes that the absorption in the two materials is equal.

Asymptotic Behavior of SP Closure

We also examine the behavior of the Su-Pomraning closure in the asymptotic regime considered by Vasques and Yadav [9] in which $\Sigma_{t,i}$ and Λ_i are $O(1)$ and $\Sigma_{a,i} = \epsilon^2\sigma_{a,i}$, i.e. $O(\epsilon^2)$. Under these assumptions, we find that

$$\Theta_{SP} \sim \frac{1}{\epsilon} \frac{\sqrt{\frac{\langle\Sigma_t\rangle}{\langle\sigma_a\rangle}}}{1 + \left(\frac{\langle\Sigma_t\rangle}{\langle\sigma_a\rangle}\right)^2 \left(\frac{\sigma_{a,1}-\sigma_{a,0}}{\Sigma_{t,1}-\Sigma_{t,0}}\right)^2} \quad , \tag{19}$$

and is therefore $O(1/\epsilon)$, because the other quantities in the expression are $O(1)$. The asymptotic analysis of Vasques and Yadav demonstrates that closure multipliers Θ that are asymptotically $O(1/\epsilon)$ result in equations that asymptotically limit to the correct diffusion equation, Eq. (13). Because Θ_{SP} is $O(1/\epsilon)$, we expect that the LP model with the Su-Pomraning closure, Eq. (8), will limit to the correct diffusion equation, Eq. (13), for the physical system under consideration.

Monte Carlo Algorithms

A detailed description of the Monte Carlo LP and LPLRP algorithms is given elsewhere [4] and will be omitted here for brevity. The SP and VY closures can be directly incorporated into the LP and LPLRP algorithms by introducing the general multiplier Θ when sampling the distance to material interface. A distance to material interface in material i, λ_i, is sampled using the distribution

$$f_i^{\Theta}(\lambda_i) = \frac{\Theta}{\Lambda_i} \exp\left(-\frac{\Theta\lambda_i}{\Lambda_i}\right) \quad . \tag{20}$$

We refer to the modified versions of the LP and LPLRP algorithms that incorporate the SP and VY closures (Eqs. (8) and (16), respectively) as LP-SP, LP-VY, and LPLRP-SP. Because the SP closure is more general than the VY closure, we only investigate the use of the SP closure with the LPLRP algorithm.

NUMERICAL RESULTS

We investigate the accuracy of the Monte Carlo LP, LP-VY, LP-SP, LPLRP, and LPLRP-SP algorithms using the set of diffusive benchmark problems defined in [9]. The transport problems involve a binary stochastic system with total width given by $2X = (\Lambda_0 + \Lambda_1)M$, where $M = 1/\epsilon$. The material parameters are given by

$$\Sigma_t(x) = \Sigma_{t,i} \quad , \quad \Sigma_a(x) = \frac{\Sigma_{a,i}}{M^2} \quad , \quad Q(x) = \frac{Q_i}{M^2} \quad , \tag{21}$$

and the system has vacuum boundary conditions at $x \pm X$. Three sets of problem parameters are defined as shown in Table I. These parameters are meant to be representative of the assumptions used in the asymptotic analysis above: Λ_i, $\Sigma_{t,i}$, $\sigma_{a,i}$, and q_i are all $O(1)$ quantities, $\Sigma_{a,i}$ and Q_i are $O(\epsilon^2)$ quantities, and X is $O(1/\epsilon)$. As ϵ decreases, or conversely as M increases, the system approaches the diffusive limit considered in the asymptotic analysis. This diffusive test problem suite has material one chosen to be a void; solid-void binary stochastic media are relevant to pebble bed reactors and atmospheric clouds [9].

Each Monte Carlo simulation was performed using 10^6 particle histories, resulting in typical pointwise relative standard deviations for ensemble-averaged scalar flux distributions of approximately 0.1-0.2%. The ensemble-averaged scalar flux distributions were tallied in the Monte Carlo simulations using uniform spatial zones of $\Delta x = 0.1$.

For each set of parameters, Vasques and Yadav [9] tabulate the benchmark, LP, and LP-VY (adjusted LP) ensemble-averaged scalar flux at the center of the system, $\langle\phi(x = 0)\rangle$. The results computed using the Monte Carlo LP and LPLRP algorithms and the SP and VY closures considered in this paper are shown in Table II. We note that the LP and LP-VY scalar flux values typically agree with those in [9] (obtained using a deterministic method) to within two standard deviations, providing an independent check on our numerical implementation. We compare the accuracy of the ensemble-averaged scalar flux values computed using the Monte Carlo algorithms to the benchmark values in [9] using relative errors computed as

$$E_{\langle\phi(x=0)\rangle} = \frac{\langle\phi(x = 0)\rangle_{MC} - \langle\phi(x = 0)\rangle_{Benchmark}}{\langle\phi(x = 0)\rangle_{Benchmark}} \quad . \tag{22}$$

We first observe that the LP ensemble-averaged scalar flux values are significantly in error by approximately 13-25%, confirming that the LP approximation does not limit to the correct diffusion result. Both the LP-VY and LP-SP algorithms are significantly more accurate than the LP approximation, with relative errors on the order of 1%. As expected given the asymptotic analysis, these numerical results confirm that the LP-VY and LP-SP algorithms limit to the correct diffusion result. The LPLRP algorithm is slightly more accurate than the LP algorithm, although this algorithm continues to exhibit errors on the order of 10-20%. Although a formal asymptotic analysis does not exist, our computational results suggest that, like the LP algorithm, the LPLRP algorithm does not limit to the correct diffusion result. Finally, the LPLRP-SP algorithm exhibits accuracy similar to the LP-VY and LP-SP algorithms, with relative errors on the order of 1%.

TABLE I: Parameters for Diffusive Test Problem Suite

Set	Λ_0	Λ_1	$\Sigma_{t,0}$	$\sigma_{a,0}$	q_0	$\Sigma_{t,1}$	$\sigma_{a,1}$	q_1
A	1.0	0.5						
B	1.0	1.0	1.0	0.1	0.2	0	0	0
C	0.5	1.0						

TABLE II: Ensemble-Averaged Scalar Flux $\langle\phi(x)\rangle$ and Relative Error at $x = 0$

		$\langle\phi(x=0)\rangle$						Relative Error (%)				
Set	M	Benchmark	LP	LP-VY	LP-SP	LPLRP	LPLRP-SP	LP	LP-VY	LP-SP	LPLRP	LPLRP-SP
A	20	0.0836	0.0729	0.0827	0.0823	0.0751	0.0829	-12.8	-1.0	-1.5	-10.2	-0.8
	40	0.0776	0.0678	0.0780	0.0777	0.0698	0.0778	-12.6	0.5	0.1	-10.0	0.2
	60	0.0758	0.0659	0.0761	0.0762	0.0682	0.0760	-13.1	0.4	0.6	-10.0	0.2
B	20	0.0816	0.0639	0.0826	0.0823	0.0675	0.0821	-21.7	1.2	0.8	-17.3	0.6
	40	0.0767	0.0587	0.0776	0.0772	0.0622	0.0774	-23.5	1.2	0.7	-18.9	1.0
	60	0.0758	0.0569	0.0759	0.0757	0.0605	0.0761	-24.9	0.2	-0.1	-20.2	0.4
C	20	0.0238	0.0195	0.0240	0.0239	0.0202	0.0240	-17.9	1.0	0.3	-15.1	0.7
	40	0.0210	0.0167	0.0212	0.0212	0.0173	0.0212	-20.7	1.1	0.9	-17.5	0.8
	60	0.0204	0.0158	0.0204	0.0204	0.0164	0.0203	-22.7	-0.1	-0.2	-19.7	-0.6

CONCLUSIONS

We demonstrated that the SP closure has the correct asymptotic limit for the diffusive physical system under investigation in this paper and that the VY closure is a special case of the SP closure obtained by assuming equal absorption in the two materials. Both of these closures are readily implemented in the Monte Carlo LP and LPLRP algorithms for particle transport in BSM. Through numerical comparisons to a diffusive benchmark suite, we confirmed that 1) the LP and LPLRP algorithms do not limit to the appropriate diffusion solution and 2) the LP-VY, LP-SP, and LPLRP-SP algorithms limit to the appropriate diffusion solution and are of comparable accuracy.

The LPLRP algorithm has been shown to be generally more accurate than the LP algorithm for non-diffusive problems [3, 4, 7]. However, the numerical results in this paper indicate that the LPLRP algorithm does not limit to the correct diffusion equation for the asymptotic limit under consideration. The work in this paper demonstrates that the SP algorithm does limit to the correct diffusion equation for the asymptotic limit considered. Future work will investigate the possibility of whether the LPLRP-SP algorithm is accurate for both diffusive and non-diffusive problems.

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